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**Cerda et al.**

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(54) **METHODS AND APPARATUS FOR IDENTIFICATION OF POLYMERIC SPECIES FROM MASS SPECTROMETRY OUTPUT**

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(57) **ABSTRACT**

(51) **Int. Cl.**  
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**G06F 19/00** (2011.01)

Methods and apparatus are provided for the identification of one or more candidate chemical formulas from mass spectrometry data corresponding to an unidentified chemical compound. By restricting the generation of candidate formulas to those having repeating units and/or end units with specified limitations, the methods and apparatus may more efficiently iteratively search for a chemical formula having matching mass spectrometry output within a threshold tolerance. In another aspect, methods and apparatus are provided for the identification of one or more candidate chemical formulas from mass spectrometry data based at least in part upon neutral loss.

(52) **U.S. Cl.**  
CPC ..... **G01N 27/62** (2013.01); **G06F 19/703** (2013.01); **G06F 19/705** (2013.01); **Y10T 436/24** (2015.01)

(58) **Field of Classification Search**  
CPC ..... G01N 30/88; G01N 2030/885; G01N 2030/8831; G01N 27/62; Y10T 436/24; G06F 19/703; G06F 19/705

See application file for complete search history.

**25 Claims, 20 Drawing Sheets**

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